

/ Transformers and Attention:  
ID22223 Scalable Machine  
Learning and Deep Learning

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November 25, 2020

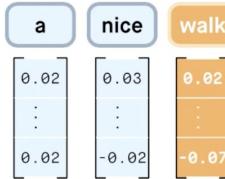


# Roadmap



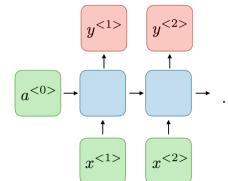
01

## Contextualized Embeddings



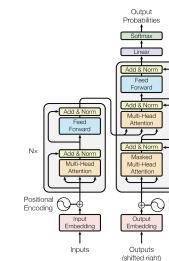
02

## From RNNs to Transformers



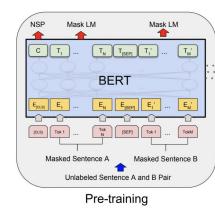
03

## Transformers Step-by-Step



04

## BERT



05

## Distillation and Practical Example



TensorFlow



# Acknowledgements

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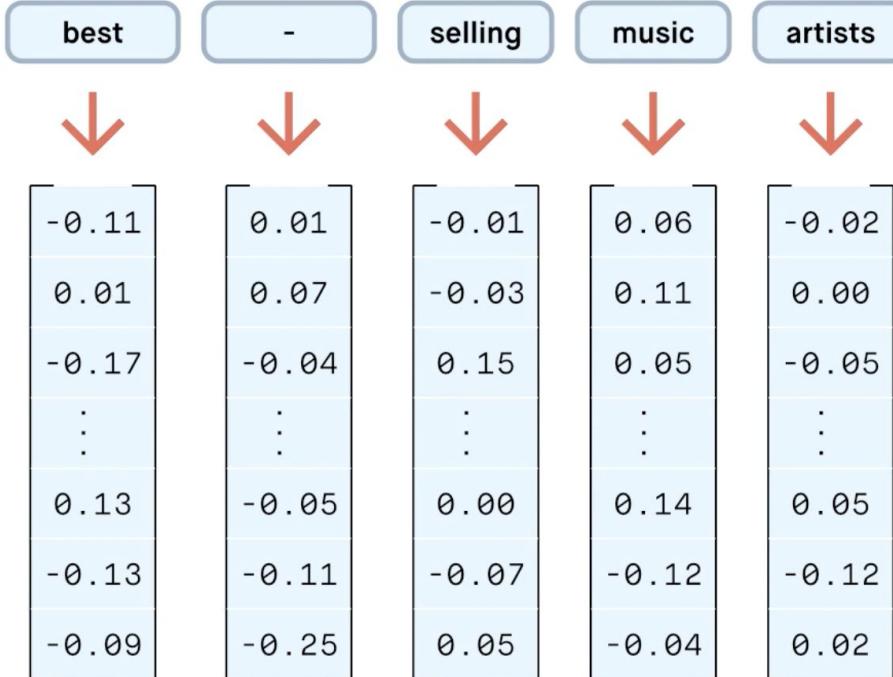
Material based on:

- Christoffer Manning's [NLP Lectures at Stanford](#)
- [The Illustrated Transformer](#) by Jay Alammar
- [Slides](#) from Jacob Devlin
- [Self-attention Video](#) from Peltarion

# 01 / Contextualized Embeddings

# Background to Natural Language Processing (NLP)

- **Word embeddings** are the basis of NLP
- Popular embeddings like **GloVe** and **Word2Vec** are pre-trained on large text corpuses based on **co-occurrence statistics**
- “A word is characterized by the company it keeps” [Firth, 1957]



[Peltarion, 2020]



# Word Embeddings



## Numerical operations

$$\begin{array}{ccccc} \text{king} & + & \text{woman} & - & \text{man} \\ \text{singing} & + & \text{yesterday} & - & \text{today} \\ \text{italy} & & \text{paris} & & \text{rome} \\ \downarrow & & \downarrow & & \downarrow \\ \begin{bmatrix} -0.04 \\ \vdots \\ 0.01 \end{bmatrix} & + & \begin{bmatrix} -0.02 \\ \vdots \\ -0.04 \end{bmatrix} & - & \begin{bmatrix} -0.03 \\ \vdots \\ -0.01 \end{bmatrix} \end{array}$$

## Semantic match

$$\approx \begin{array}{c} \text{queen} \\ \approx \text{sang} \\ \approx \text{france} \\ \approx \begin{bmatrix} -0.04 \\ \vdots \\ 0.01 \end{bmatrix} \end{array}$$

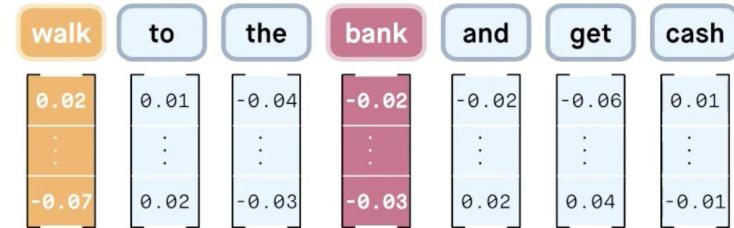
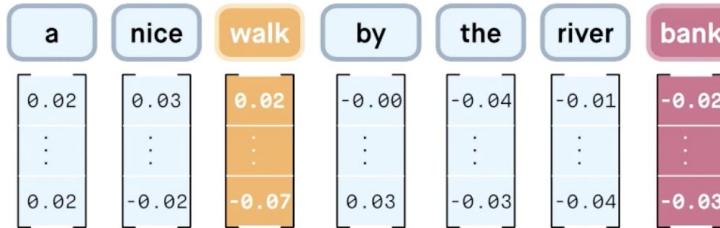
# Word Embeddings

**Problem:** Word embeddings are **context-free**

a	nice	walk	by	the	river	bank
0.02	0.03	0.02	-0.00	-0.04	-0.01	-0.02
:	:	:	:	:	:	:
0.02	-0.02	-0.07	0.03	-0.03	-0.04	-0.03

walk	to	the	bank	and	get	cash
0.02	0.01	-0.04	-0.02	-0.02	-0.06	0.01
:	:	:	:	:	:	:
-0.07	0.02	-0.03	-0.03	0.02	0.04	-0.01

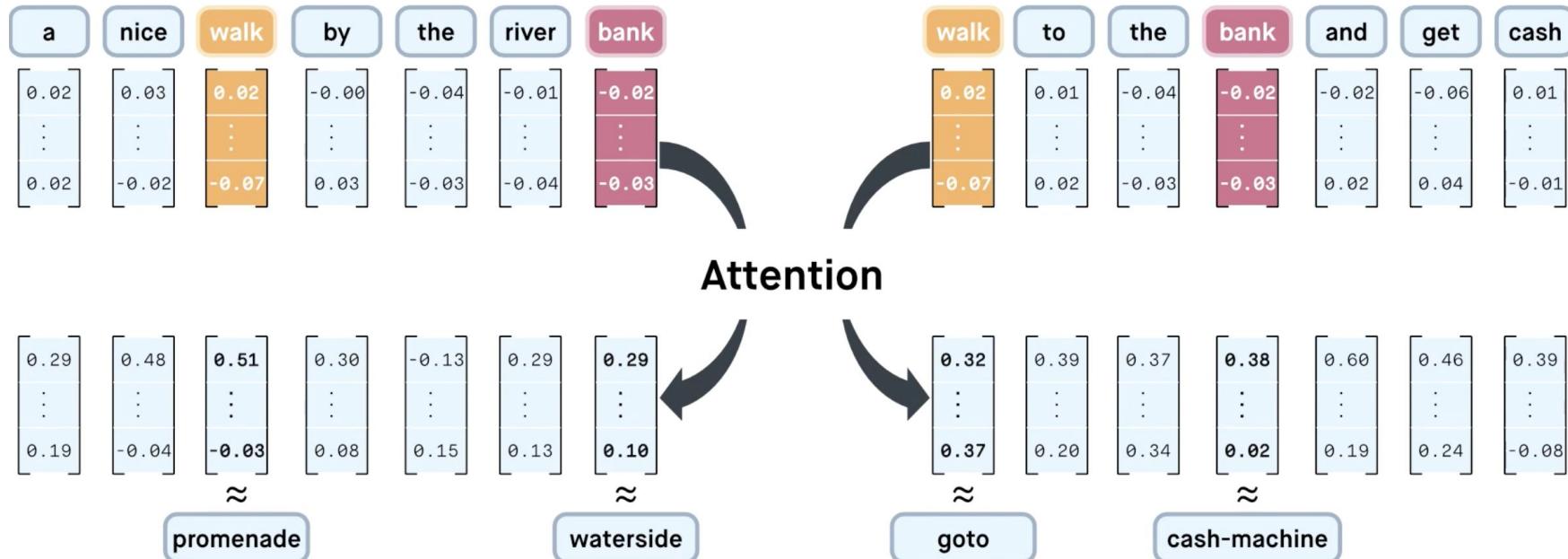
**Problem:** Word embeddings are **context-free**



# Word Embeddings

**Problem:** Word embeddings are **context-free**

**Solution:** Create **contextualized** representation



## 02 / From RNNs to Transformers

# Problems with RNNs - Motivation for Transformers

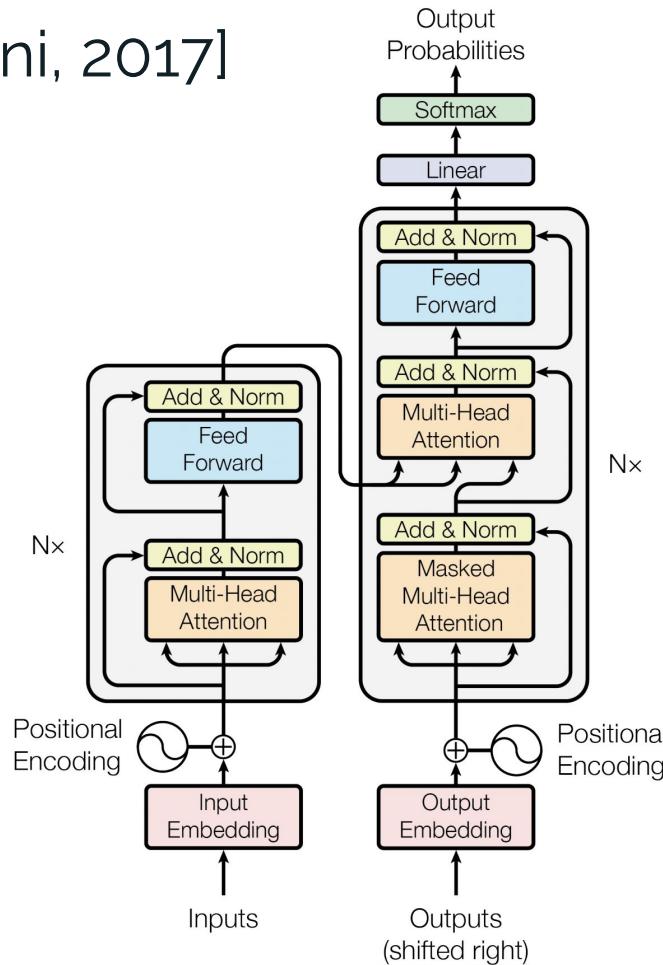
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- Sequential computations **prevents parallelization**
- Despite GRUs and LSTMs, RNNs still need attention mechanisms to deal with **long range dependencies**
- Attention gives us access to any state... Maybe we don't need the costly recursion? 🤔
- Then NLP can have deep models, solves our computer vision envy!



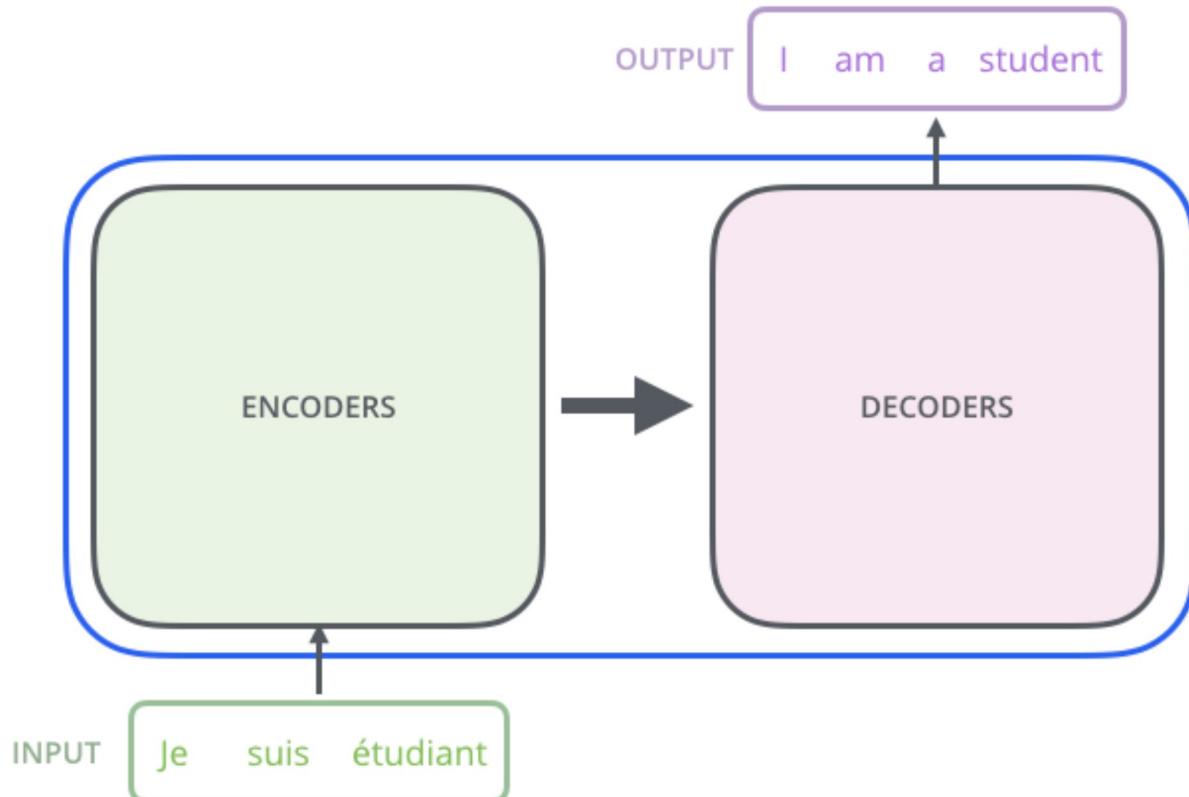
# Attention is all you need! [Vaswani, 2017]

- Sequence-to-sequence model for Machine Translation
- **Encoder-decoder** architecture
- Multi-headed **self-attention**
  - Models context and no locality bias



## 03 / Transformers Step-by-Step

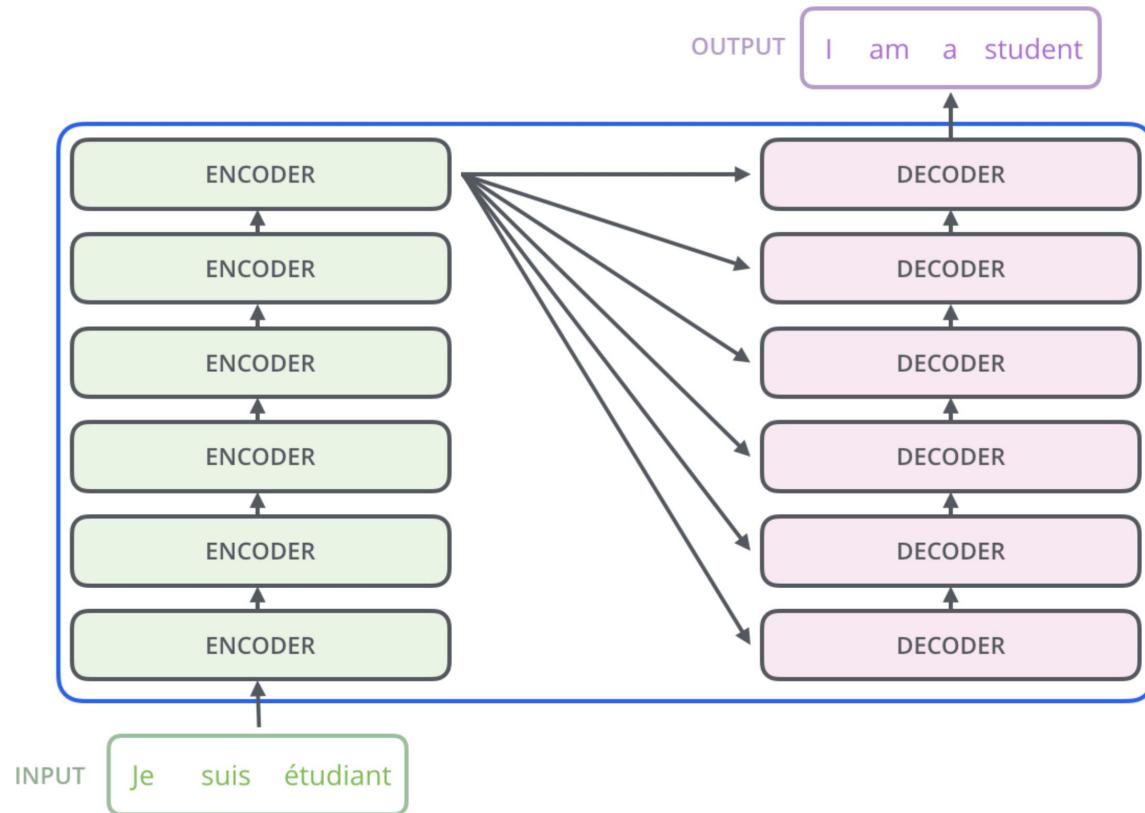
# Understanding the Transformer: Step-by-Step



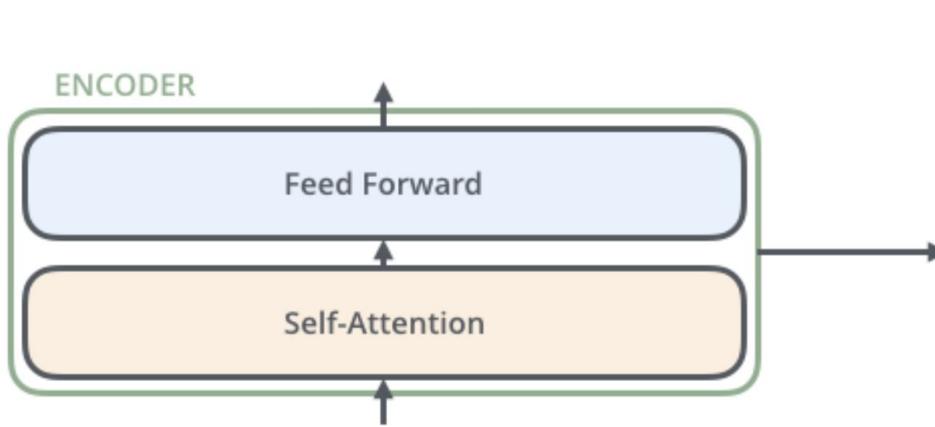
# Understanding the Transformer: Step-by-Step

No recursion, instead  
**stacking encoder** and  
**decoder** blocks

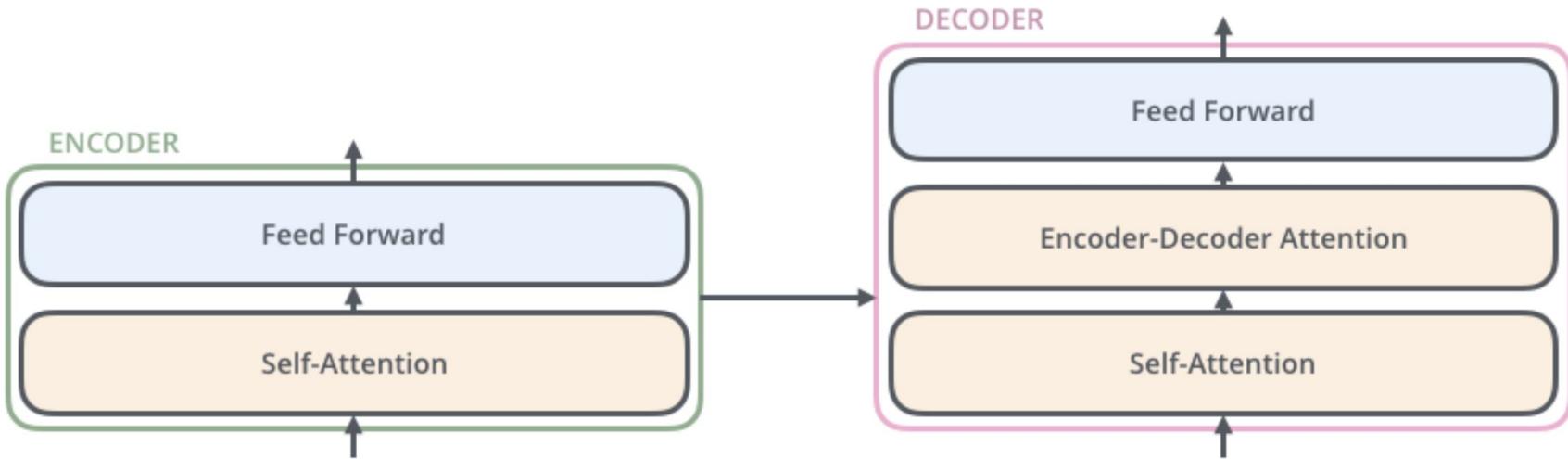
- Originally: 6 layers
- BERT base: 12 layers
- BERT large: 24 layers
- GPT2-XL: 48 layers
- GPT3: 96 layers



# The Encoder Block



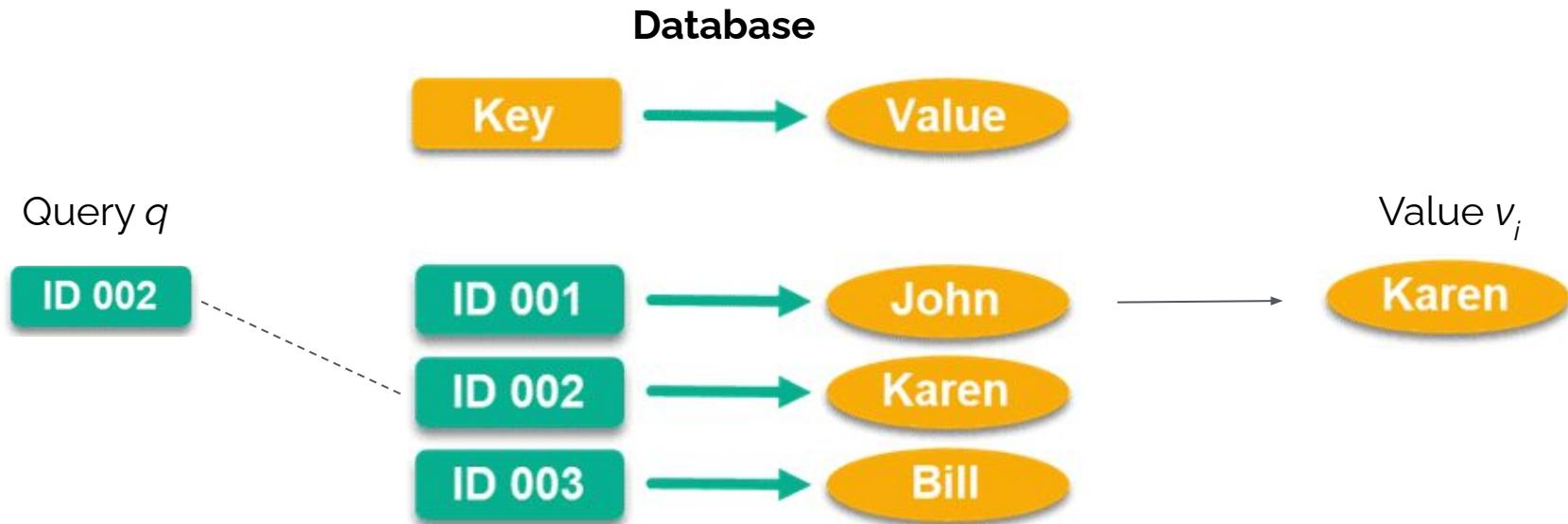
# The Encoder and Decoder Blocks



# II Attention Preliminaries



Mimics the retrieval of a value  $v_i$  for a query  $q$  based on a key  $k_i$  in a database, but in a probabilistic fashion



# Dot-Product Attention

- Queries, keys and values are vectors
- Output is a **weighted sum** of the values
- Weights are computed as the **scaled dot-product** (similarity) between the query and the keys

$$\text{Attention}(q, K, V) = \sum_i \text{Similarity}(q, k_i) \cdot v_i = \sum_i \frac{e^{q \cdot k_i / \sqrt{d_k}}}{\sum_j e^{q \cdot k_j / \sqrt{d_k}}} v_i$$

Output is a  
row-vector

- Can stack multiple queries into a matrix  $Q$

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

Output is again  
a matrix

- Self-attention: Let the word embeddings be the queries, keys and values, i.e. **let the words select each other**



# Self-Attention Mechanism

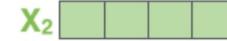
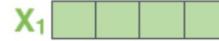


Input

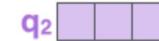
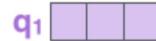
Thinking

Machines

Embedding

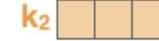
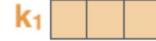


Queries



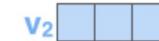
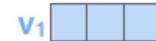
$W^Q$

Keys

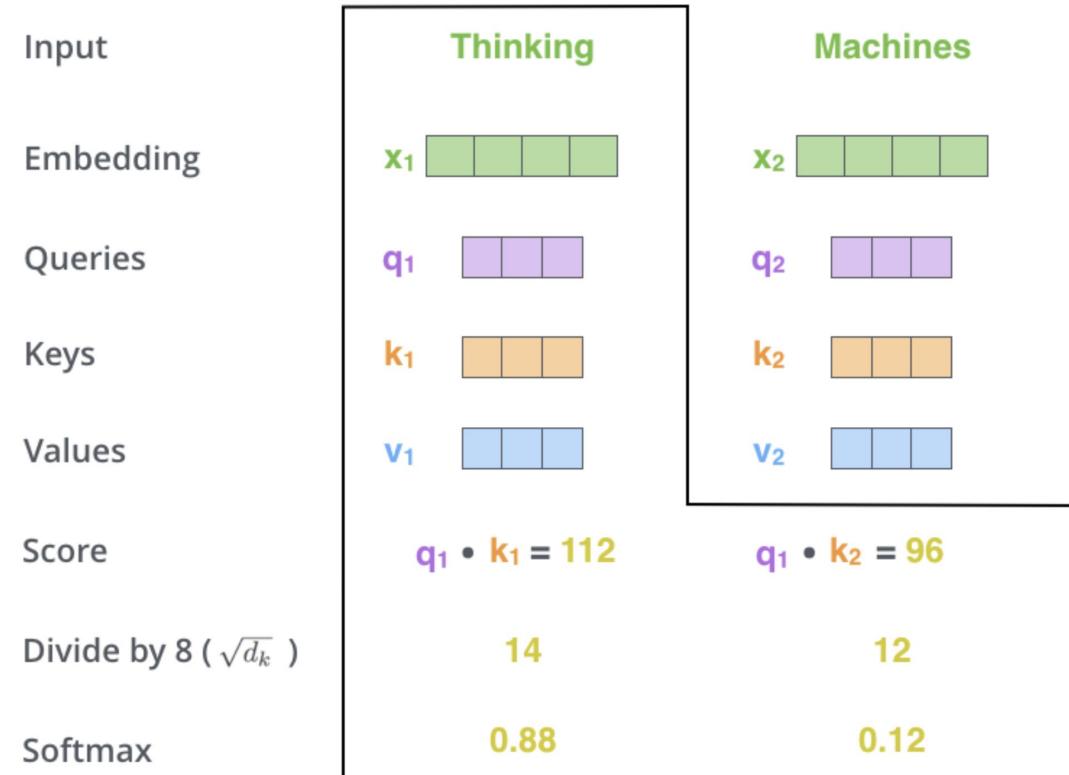


$W^K$

Values



$W^V$



# Self-Attention Mechanism in Matrix Notation

$$\mathbf{X} \times \mathbf{W}^Q = \mathbf{Q}$$

A green input matrix  $\mathbf{X}$  (3x3) is multiplied by a purple weight matrix  $\mathbf{W}^Q$  (3x3) to produce a purple output matrix  $\mathbf{Q}$  (3x3).

$$\mathbf{X} \times \mathbf{W}^K = \mathbf{K}$$

A green input matrix  $\mathbf{X}$  (3x3) is multiplied by an orange weight matrix  $\mathbf{W}^K$  (3x3) to produce an orange output matrix  $\mathbf{K}$  (3x3).

$$\mathbf{X} \times \mathbf{W}^V = \mathbf{V}$$

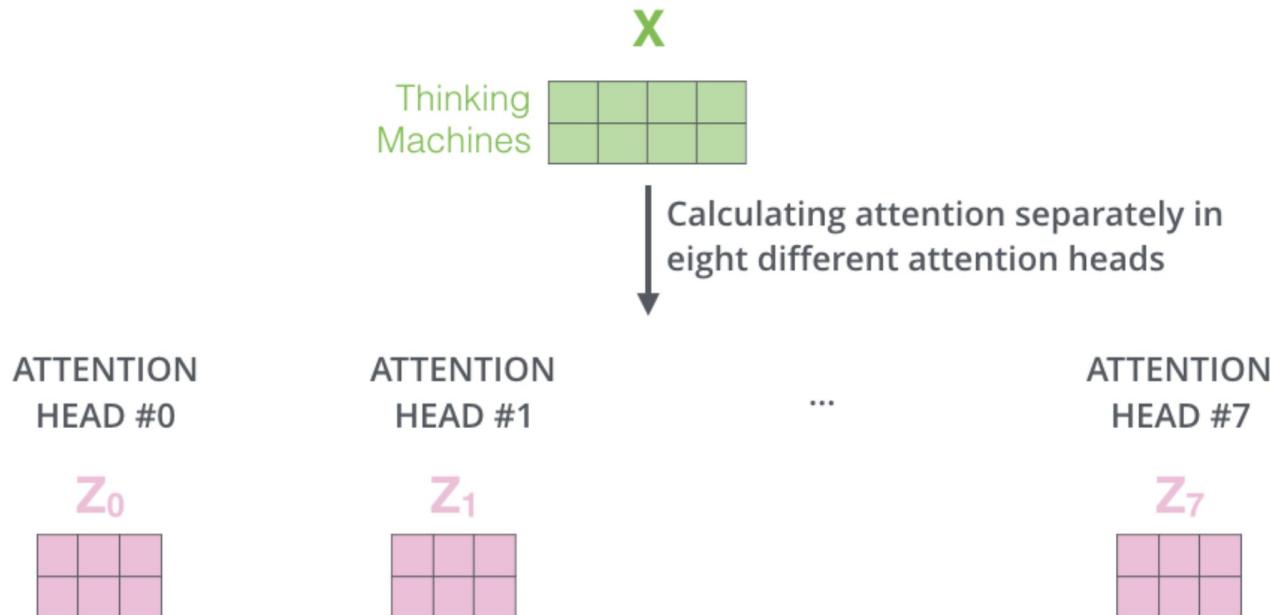
A green input matrix  $\mathbf{X}$  (3x3) is multiplied by a blue weight matrix  $\mathbf{W}^V$  (3x3) to produce a blue output matrix  $\mathbf{V}$  (3x3).

$$\text{softmax}\left(\frac{\mathbf{Q} \times \mathbf{K}^T}{\sqrt{d_k}}\right) \mathbf{V} = \mathbf{Z}$$

The matrices  $\mathbf{Q}$  (purple 3x3),  $\mathbf{K}^T$  (orange 3x3), and  $\mathbf{V}$  (blue 3x3) are multiplied sequentially to produce the final output matrix  $\mathbf{Z}$  (pink 3x3). The division by  $\sqrt{d_k}$  is shown below the multiplication.

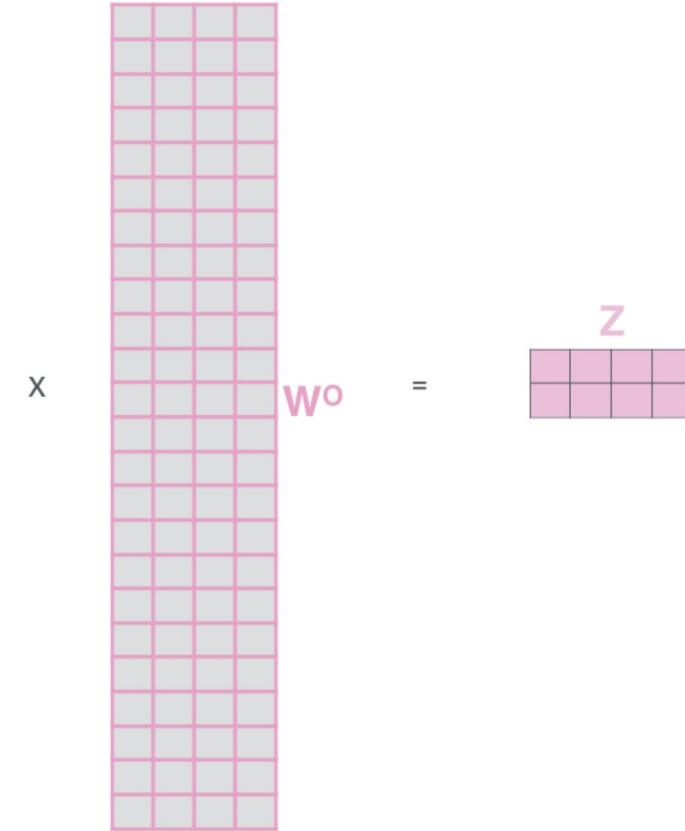
# ¶ Multi-Headed Self-Attention

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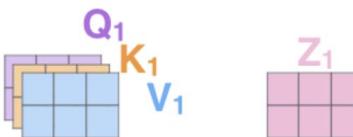
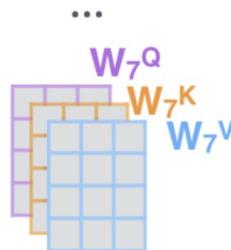
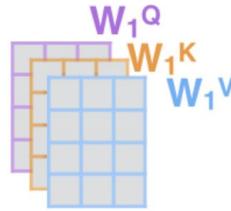
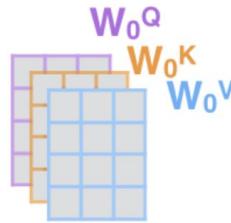
# Π Multi-Headed Self-Attention

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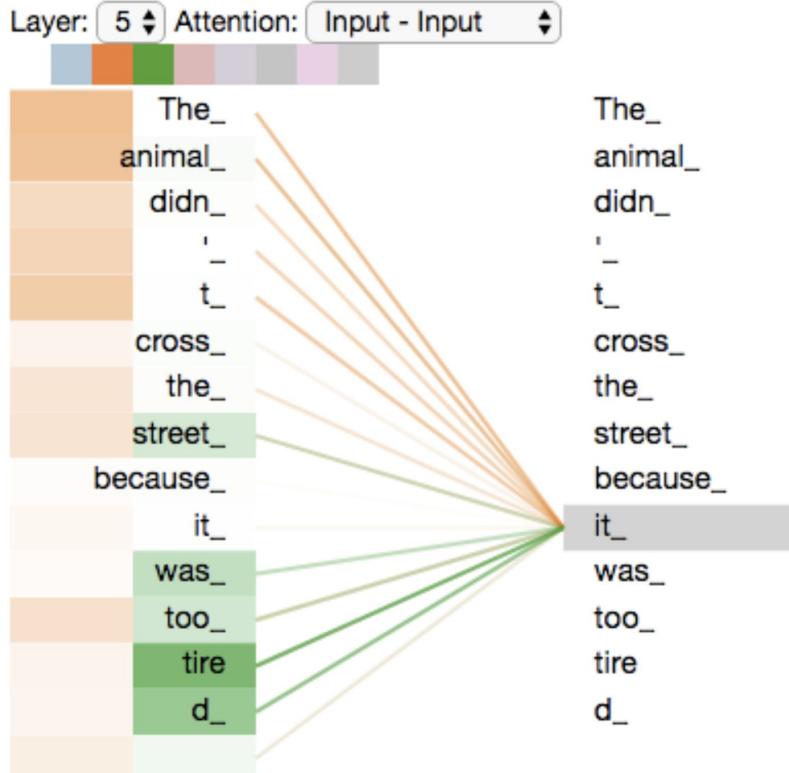
# Self-Attention: Putting It All Together

Thinking  
Machines





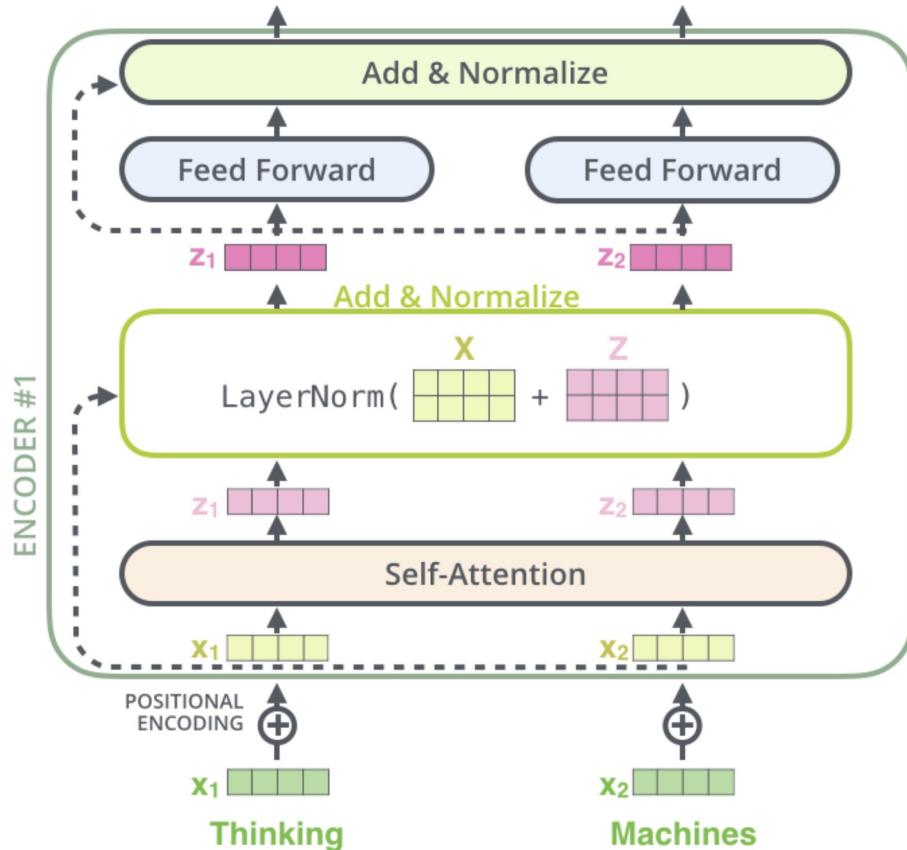
# Attention visualized



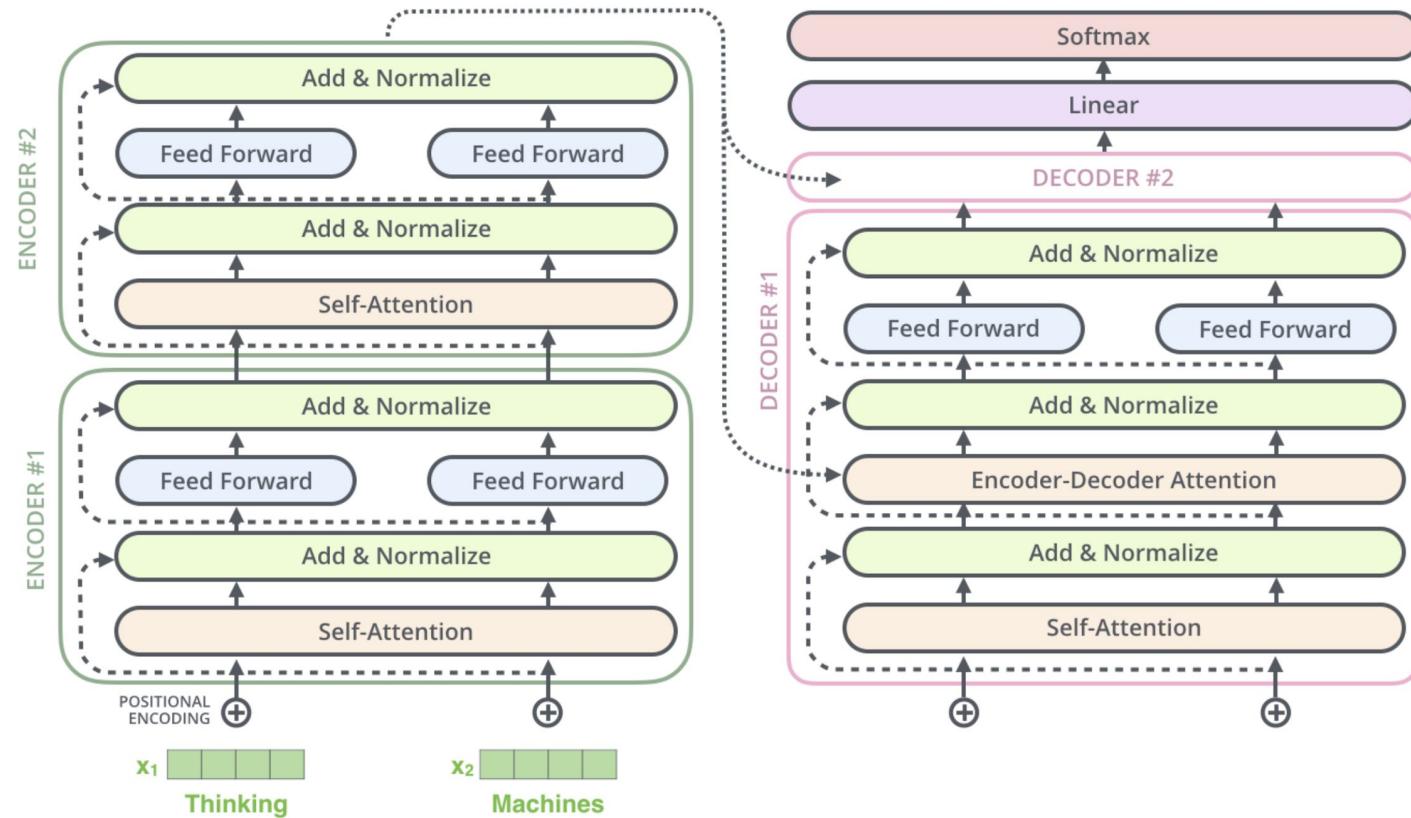
# The Full Encoder Block

Encoder block consisting of:

- Multi-headed self-attention
- Feedforward NN (FC 2 layers)
- Skip connections
- Layer normalization - Similar to batch normalization but computed over features (words/tokens) for a single sample



# Encoder-Decoder Architecture - Small Example



# Positional Encodings

- Attention mechanism has no locality bias - **no notion of word order**
- **Add positional encodings** to input embeddings to let model learn relative positioning

$$\text{PE}(\text{pos}, 2i) = \sin\left(\frac{\text{pos}}{10000^{2i/d_{\text{model}}}}\right)$$

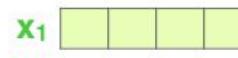
$$\text{PE}(\text{pos}, 2i + 1) = \cos\left(\frac{\text{pos}}{10000^{2i/d_{\text{model}}}}\right)$$

EMBEDDING  
WITH TIME  
SIGNAL

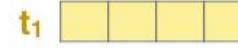
POSITIONAL  
ENCODING

EMBEDDINGS

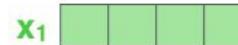
INPUT



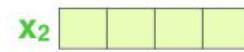
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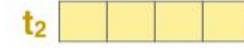
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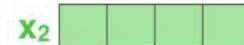
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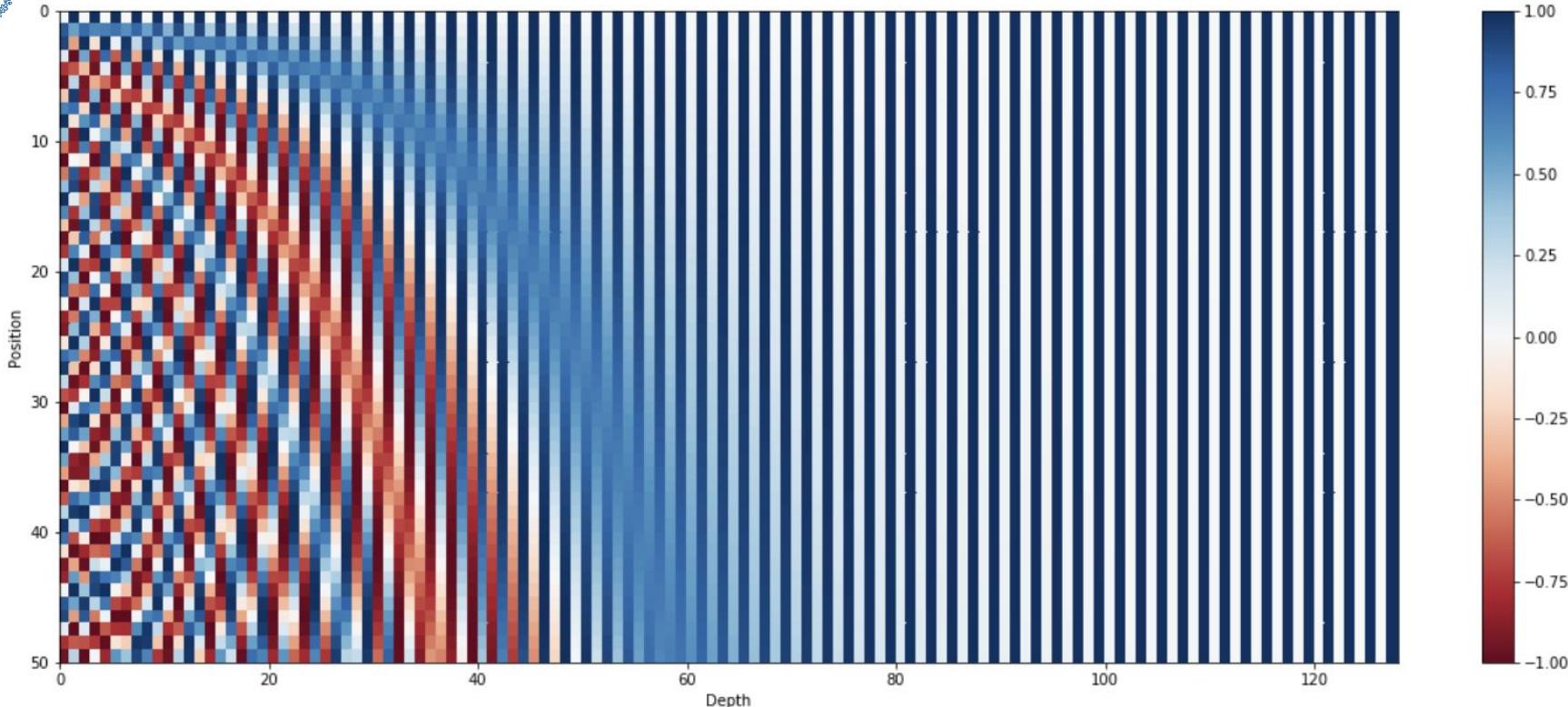
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suis



# Positional Encodings



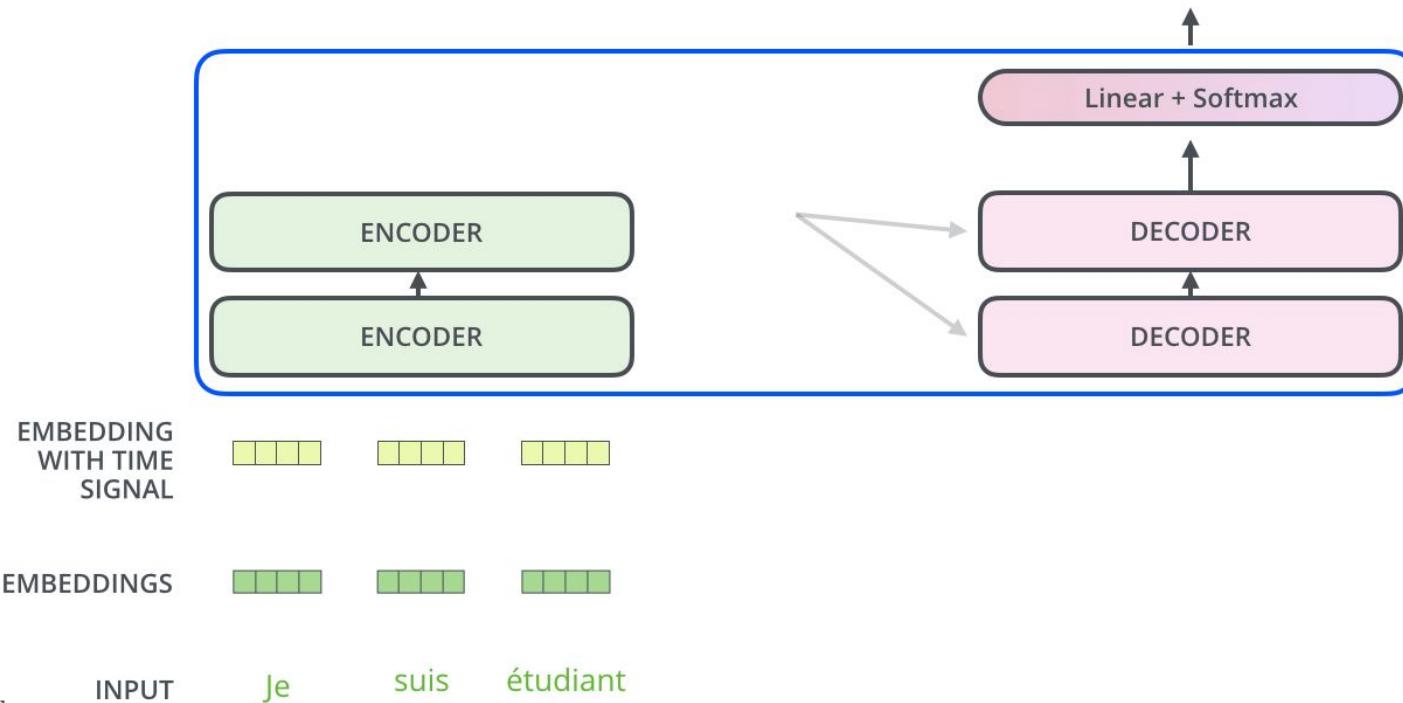


# Let's start the encoding!

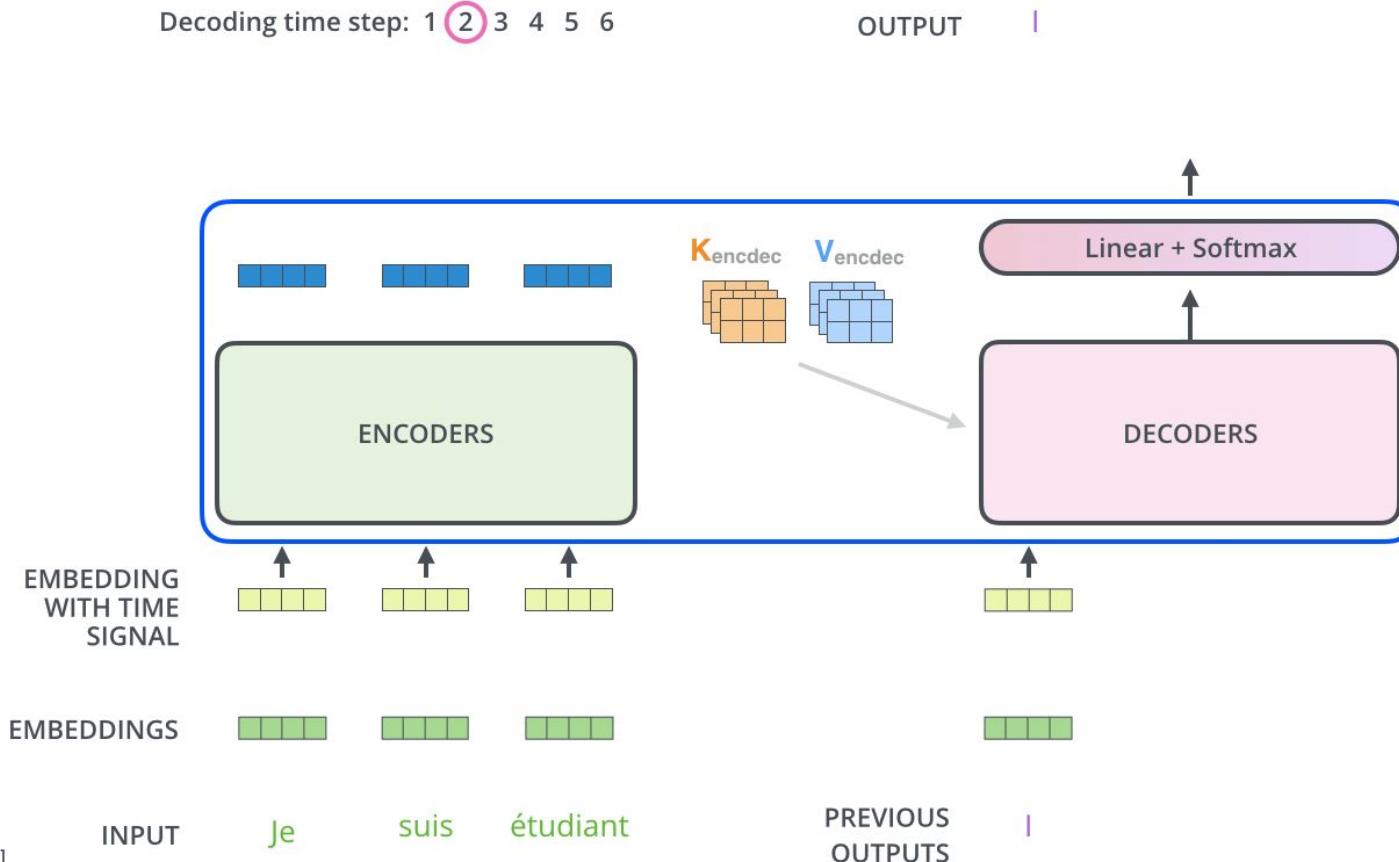


Decoding time step: 1 2 3 4 5 6

OUTPUT



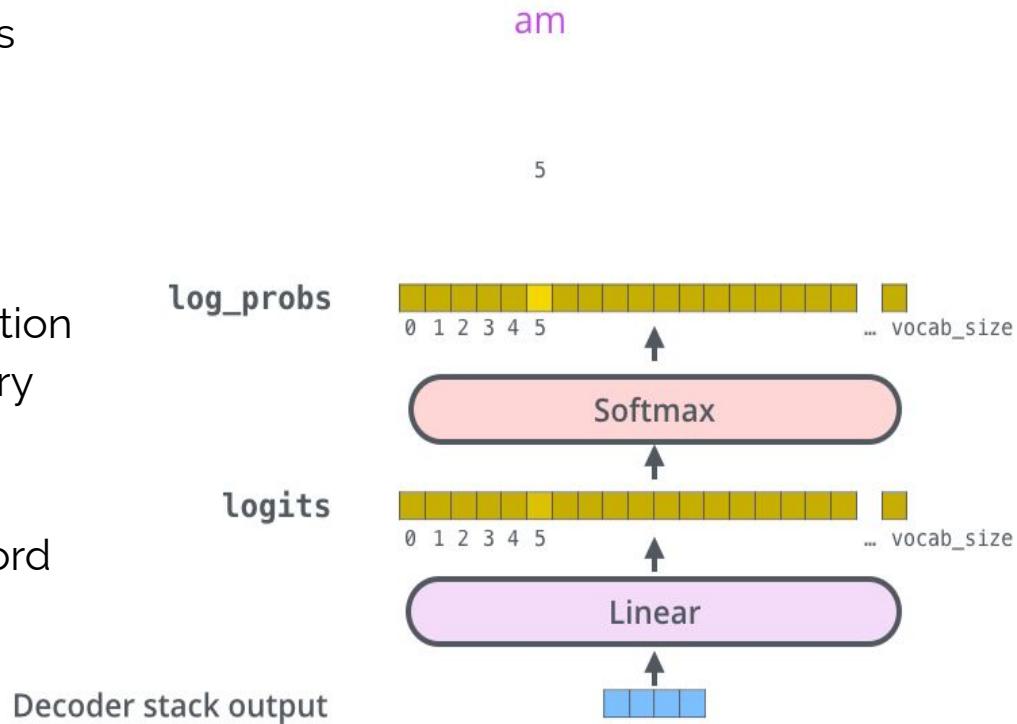
# Decoding procedure



# Producing the output text



- The output from the decoder is passed through a final fully connected **linear layer** with a **softmax** activation function
- Produces a probability distribution over the pre-defined vocabulary of output words (tokens)
- Greedy decoding** picks the word with the highest probability at each time step



## Target Model Outputs

Output Vocabulary: a am I thanks student <eos>

position #1	0.0	0.0	1.0	0.0	0.0	0.0
-------------	-----	-----	-----	-----	-----	-----

position #2	0.0	1.0	0.0	0.0	0.0	0.0
-------------	-----	-----	-----	-----	-----	-----

position #3	1.0	0.0	0.0	0.0	0.0	0.0
-------------	-----	-----	-----	-----	-----	-----

position #4	0.0	0.0	0.0	0.0	1.0	0.0
-------------	-----	-----	-----	-----	-----	-----

position #5	0.0	0.0	0.0	0.0	0.0	1.0
-------------	-----	-----	-----	-----	-----	-----

a am I thanks student <eos>

## Trained Model Outputs

Output Vocabulary: a am I thanks student <eos>

position #1	0.01	0.02	0.93	0.01	0.03	0.01
-------------	------	------	------	------	------	------

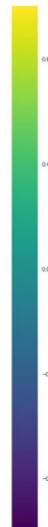
position #2	0.01	0.8	0.1	0.05	0.01	0.03
-------------	------	-----	-----	------	------	------

position #3	0.99	0.001	0.001	0.001	0.002	0.001
-------------	------	-------	-------	-------	-------	-------

position #4	0.001	0.002	0.001	0.02	0.94	0.01
-------------	-------	-------	-------	------	------	------

position #5	0.01	0.01	0.001	0.001	0.001	0.98
-------------	------	------	-------	-------	-------	------

a am I thanks student <eos>





# Complexity Comparison



Layer Type	Complexity per Layer	Sequential Operations	Maximum Path Length
Self-Attention	$O(n^2 \cdot d)$	$O(1)$	$O(1)$
Recurrent	$O(n \cdot d^2)$	$O(n)$	$O(n)$
Convolutional	$O(k \cdot n \cdot d^2)$	$O(1)$	$O(\log_k(n))$

## 04 / BERT



# BERT

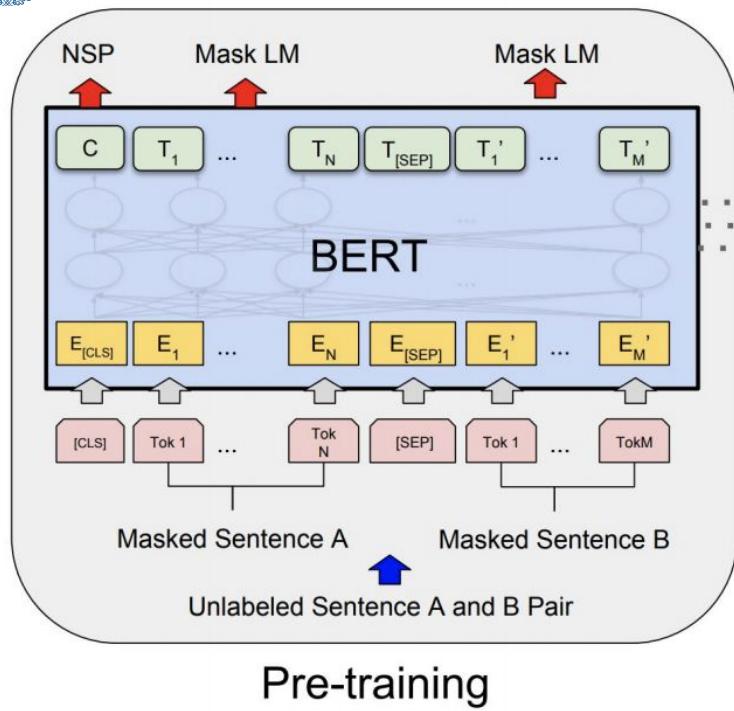


**Bidirectional Encoder Representations  
from Transformers**

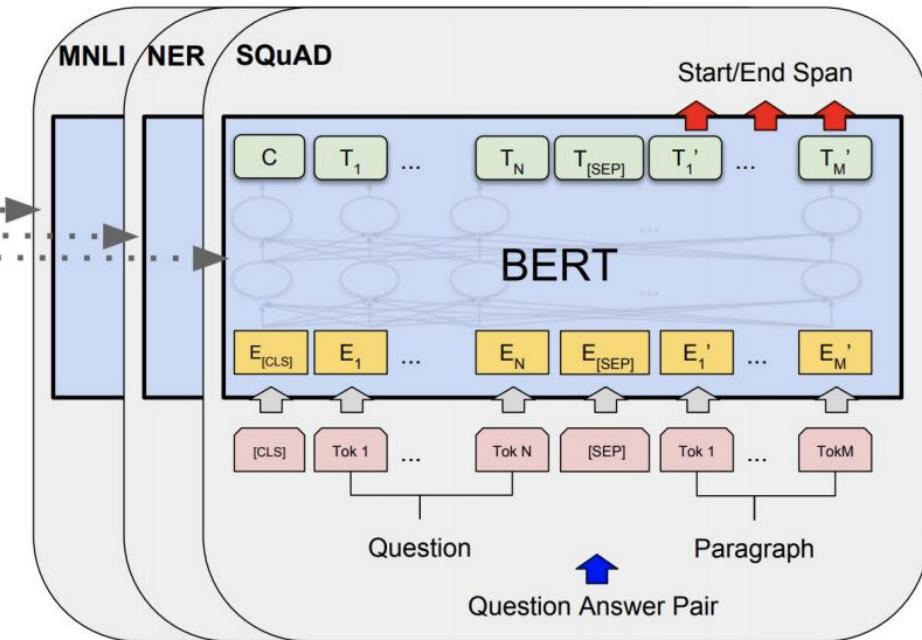
- Self-supervised **pre-training** of Transformers encoder for **language understanding**
- **Fine-tuning** for specific downstream task



# BERT Training Procedure



Pre-training



Fine-Tuning



# BERT Training Objectives



## Masked Language Modelling

the man went to the [MASK] to buy a [MASK] of milk

↑    ↑  
store    gallon

## Next Sentence Prediction

**Sentence A** = The man went to the store.

**Sentence B** = He bought a gallon of milk.

**Label** = IsNextSentence

**Sentence A** = The man went to the store.

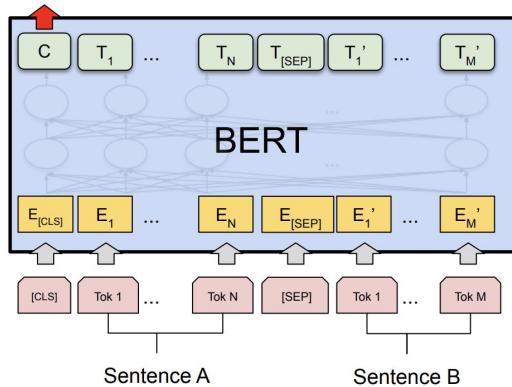
**Sentence B** = Penguins are flightless.

**Label** = NotNextSentence

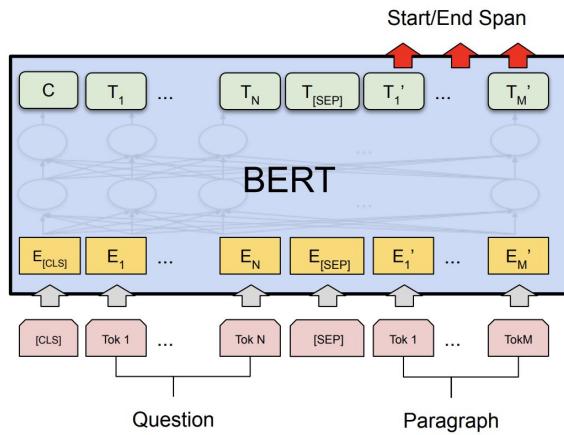
# BERT Fine-Tuning Examples



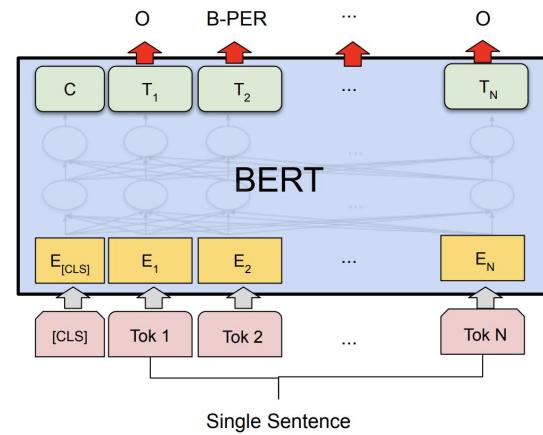
Class Label



Sentence  
Classification



Question  
Answering



Named Entity  
Recognition



# Exploring the Limits of Transfer Learning (T5)



- Scaling up **models size** and amount of **training data** helps a lot
- Best model is 11B (!!!) parameters
- Exact **pre-training objective** (MLM, NSP, corruption) doesn't matter too much
- SuperGLUE benchmark:

Rank	Name	Model	URL	Score	BoolQ	CB	COPA	MultiRC	ReCoRD	RTE	WiC	WSC	AX-b	AX-g
1	SuperGLUE Human Baselines	SuperGLUE Human Baselines		89.8	89.0	95.8/98.9	100.0	81.8/51.9	91.7/91.3	93.6	80.0	100.0	76.6	99.3/99.7
+	2 T5 Team - Google	T5		89.3	91.2	93.9/96.8	94.8	88.1/63.3	94.1/93.4	92.5	76.9	93.8	65.6	92.7/91.9
+	3 Huawei Noah's Ark Lab	NEZHA-Plus		86.7	87.8	94.4/96.0	93.6	84.6/55.1	90.1/89.6	89.1	74.6	93.2	58.0	87.1/74.4
+	4 Alibaba PAI&ICBU	PAI Albert		86.1	88.1	92.4/96.4	91.8	84.6/54.7	89.0/88.3	88.8	74.1	93.2	75.6	98.3/99.2
+	5 Tencent Jarvis Lab	RoBERTa (ensemble)		85.9	88.2	92.5/95.6	90.8	84.4/53.4	91.5/91.0	87.9	74.1	91.8	57.6	89.3/75.6
6	Zhuiyi Technology	RoBERTa-mtl-adv		85.7	87.1	92.4/95.6	91.2	85.1/54.3	91.7/91.3	88.1	72.1	91.8	58.5	91.0/78.1
7	Facebook AI	RoBERTa		84.6	87.1	90.5/95.2	90.6	84.4/52.5	90.6/90.0	88.2	69.9	89.0	57.9	91.0/78.1

## 05 / Practical Examples



# BERT in low-latency production settings



GOOGLE \ TECH \ ARTIFICIAL INTELLIGENCE

## Google is improving 10 percent of searches by understanding language context

Say hello to BERT

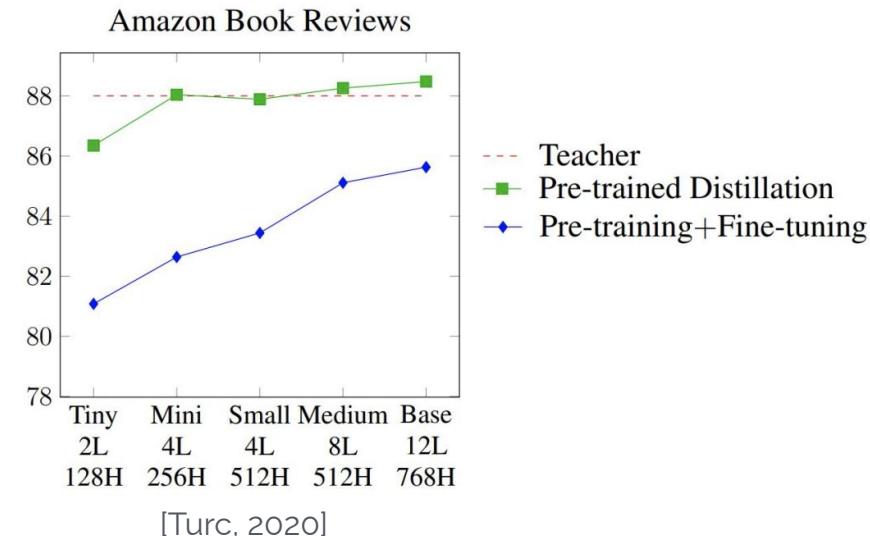
By Dieter Bohn | @backlon | Oct 25, 2019, 3:01am EDT

## Bing says it has been applying BERT since April

The natural language processing capabilities are now applied to all Bing queries globally.

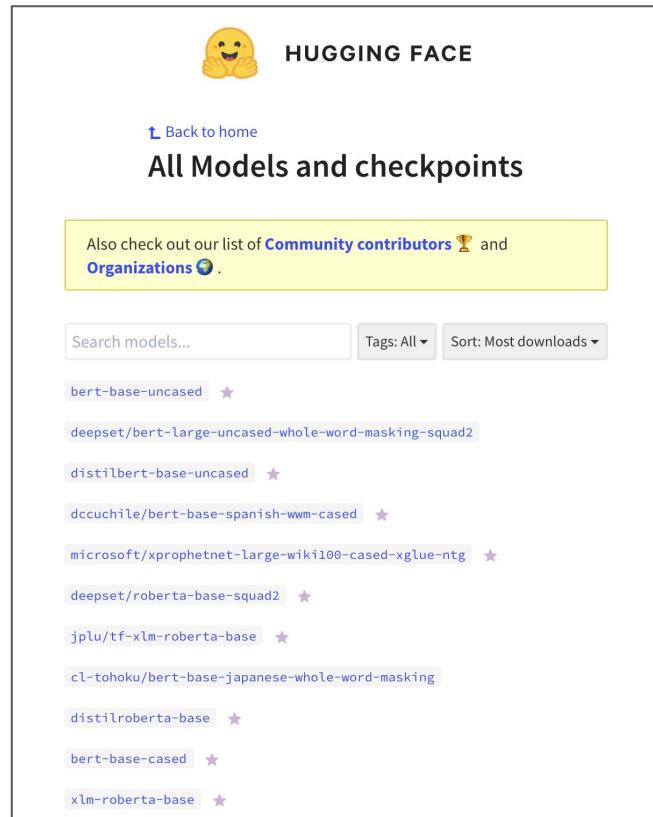
[George Nguyen](#) on November 19, 2019 at 1:38 pm

- Modern pre-trained language models are **huge** and very **computationally expensive**
- How are these companies applying them to low-latency applications?
- Distillation!
  - Train SOTA **teacher model** (pre-training + fine-tuning)
  - Train smaller **student model** that **mimics** the teacher's output on a large dataset on unlabeled data
- Why does it work so well?



# Transformers in TensorFlow using HuggingFace 😊

- The **HuggingFace Library** contains a majority of the recent pre-trained State-of-the-art NLP models, as well as over 4 000 community uploaded models
- Works with both **TensorFlow** and **PyTorch**



The screenshot shows the Hugging Face website's "All Models and checkpoints" page. At the top, there is a yellow smiley face emoji and the text "HUGGING FACE". Below that is a "Back to home" link. The main heading is "All Models and checkpoints". A callout box in the middle of the page says "Also check out our list of [Community contributors](#) 🏆 and [Organizations](#) 🌐". At the bottom, there is a search bar with "Search models...", a "Tags: All" dropdown, and a "Sort: Most downloads" dropdown. A list of model names follows:

- bert-base-uncased ★
- deepset/bert-large-uncased-whole-word-masking-squad2
- distilbert-base-uncased ★
- dccuchile/bert-base-spanish-wmm-cased ★
- microsoft/xprophetnet-large-wiki100-cased-xglue-ntg ★
- deepset/roberta-base-squad2 ★
- jplu/tf-xlm-roberta-base ★
- cl-tohoku/bert-base-japanese-whole-word-masking
- distilroberta-base ★
- bert-base-cased ★
- xlm-roberta-base ★



# Transformers in TensorFlow using HuggingFace 😊

---



```
from transformers import BertTokenizerFast, TFBertForSequenceClassification
from datasets import load_dataset
import tensorflow as tf

dataset = load_dataset("imdb").shuffle()
tokenizer = BertTokenizerFast.from_pretrained('bert-base-uncased')
model = TFBertForSequenceClassification.from_pretrained('bert-base-uncased', num_labels=2)

train_encodings = tokenizer(dataset['train']['text'], truncation=True, padding=True)
train_dataset = tf.data.Dataset.from_tensor_slices((dict(train_encodings), dataset['train']['label']))
val_dataset = ... // Analogously

optimizer = tf.keras.optimizers.Adam(learning_rate=5e-5)
model.compile(optimizer=optimizer, loss=model.compute_loss)
model.fit(train_dataset.batch(16), epochs=3, batch_size=16)

model.evaluate(val_dataset.batch(16), verbose=0)
```



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## 06 / Wrap Up

# Summary

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- Transformers have blown other architectures out of the water for NLP
- Get rid of recurrence and rely on **self-attention**
- NLP pre-training using **Masked Language Modelling**
- Most recent improvements using **larger models** and **more data**
- **Distillation** can make model serving and inference more tractable



# Questions?

/November 25, 2020

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**Thanks**

**Karl Fredrik Erliksson**

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